

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
 Data File : VU045104.D
 Acq On : 04 Oct 2021 18:18
 Operator : SY/MD
 Sample : M3974-07ME
 Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW8Z1ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045104.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	32	40	68	rBV	50768	116301	1.79%	0.679%
2	1.597	73	80	95	rVB	97255	141450	2.18%	0.826%
3	1.896	166	173	189	rBV	41458	68204	1.05%	0.398%
4	2.536	359	372	386	rBV	198281	350279	5.39%	2.045%
5	2.964	497	505	508	rBV2	542	661	0.01%	0.004%
6	3.038	519	528	537	rBV4	2385	4266	0.07%	0.025%
7	3.105	544	549	553	rBV2	224	278	0.00%	0.002%
8	3.182	564	573	588	rVB4	1325	3033	0.05%	0.018%
9	3.237	588	590	595	rBV	254	250	0.00%	0.001%
10	3.343	612	623	639	rVB3	6731	14125	0.22%	0.082%
11	3.944	802	810	813	rBV2	185	308	0.00%	0.002%
12	4.514	981	987	994	rVB3	280	431	0.01%	0.003%
13	4.665	1013	1034	1084	rBV2	347474	1066883	16.43%	6.228%
14	5.067	1142	1159	1185	rBV	198897	483710	7.45%	2.824%
15	5.288	1224	1228	1229	rBV2	378	303	0.00%	0.002%
16	5.375	1249	1255	1262	rVB4	569	789	0.01%	0.005%
17	5.427	1267	1271	1275	rBV2	221	263	0.00%	0.002%
18	5.536	1300	1305	1311	rBV2	222	257	0.00%	0.002%
19	5.723	1342	1363	1393	rBV2	473513	1223544	18.85%	7.143%
20	5.906	1417	1420	1429	rVB3	313	460	0.01%	0.003%
21	5.983	1429	1444	1473	rBV4	8435	23015	0.35%	0.134%
22	6.160	1493	1499	1501	rBV	232	315	0.00%	0.002%
23	6.189	1501	1508	1512	rBV4	271	414	0.01%	0.002%
24	6.250	1512	1527	1556	rVV	373041	772461	11.90%	4.510%
25	6.375	1563	1566	1569	rVB2	351	252	0.00%	0.001%
26	6.542	1601	1618	1650	rBV	3341005	6492665	100.00%	37.903%
27	6.694	1652	1665	1691	rVB	271456	576366	8.88%	3.365%
28	6.874	1716	1721	1724	rBV	225	255	0.00%	0.001%
29	6.906	1728	1731	1735	rVB	306	241	0.00%	0.001%
30	7.050	1772	1776	1779	rBV3	293	329	0.01%	0.002%
31	7.195	1809	1821	1822	rBV3	2583	3394	0.05%	0.020%
32	7.349	1864	1869	1871	rBV	274	236	0.00%	0.001%
33	7.404	1880	1886	1889	rBV2	215	263	0.00%	0.002%
34	7.571	1922	1938	1965	rBV	140061	279120	4.30%	1.629%
35	7.693	1969	1976	1986	rBV3	1201	2277	0.04%	0.013%
36	7.800	2005	2009	2012	rBV2	250	249	0.00%	0.001%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

37	7.816	2012	2014	2020	rVB	369	337	0.01%	0.002%
38	7.851	2020	2025	2026	rBV2	248	250	0.00%	0.001%
39	7.902	2026	2041	2056	rBV	495355	910804	14.03%	5.317%
40	7.973	2057	2063	2076	rVB	12124	20286	0.31%	0.118%
41	8.185	2116	2129	2154	rBV3	83405	187208	2.88%	1.093%
42	8.472	2211	2218	2226	rVB2	483	841	0.01%	0.005%
43	8.555	2234	2244	2256	rBV3	20914	36222	0.56%	0.211%
44	8.671	2260	2280	2314	rBV	387049	849882	13.09%	4.962%
45	9.427	2500	2515	2535	rBV	474502	958639	14.76%	5.596%
46	9.574	2553	2561	2572	rVB2	2822	4497	0.07%	0.026%
47	9.703	2592	2601	2612	rVB2	2576	4174	0.06%	0.024%
48	9.835	2635	2642	2649	rBV2	262	436	0.01%	0.003%
49	10.111	2720	2728	2734	rBV	1226	1970	0.03%	0.012%
50	10.401	2814	2818	2822	rBV2	345	415	0.01%	0.002%
51	10.478	2840	2842	2845	rBV	326	265	0.00%	0.002%
52	10.536	2854	2860	2864	rBV3	561	595	0.01%	0.003%
53	10.674	2894	2903	2911	rVB3	2735	3895	0.06%	0.023%
54	10.771	2919	2933	2953	rVB	437424	713241	10.99%	4.164%
55	10.867	2957	2963	2967	rBV3	556	607	0.01%	0.004%
56	10.899	2970	2973	2984	rVB5	840	1339	0.02%	0.008%
57	11.012	3001	3008	3011	rVV3	310	433	0.01%	0.003%
58	11.028	3011	3013	3020	rVB2	447	437	0.01%	0.003%
59	11.118	3029	3041	3048	rBV6	1850	3252	0.05%	0.019%
60	11.243	3076	3080	3085	rBV2	256	265	0.00%	0.002%
61	11.298	3090	3097	3107	rVB3	393	594	0.01%	0.003%
62	11.417	3130	3134	3141	rBV4	772	1101	0.02%	0.006%
63	11.465	3141	3149	3150	rBV4	2316	2712	0.04%	0.016%
64	11.581	3176	3185	3189	rBV4	635	799	0.01%	0.005%
65	11.652	3203	3207	3213	rVB3	498	591	0.01%	0.003%
66	11.700	3214	3222	3229	rBV4	1912	2868	0.04%	0.017%
67	11.822	3246	3260	3286	rVV	558568	884061	13.62%	5.161%
68	11.976	3304	3308	3319	rVB4	2282	3493	0.05%	0.020%
69	12.060	3330	3334	3337	rBV2	317	254	0.00%	0.001%
70	12.201	3358	3378	3393	rBV	523581	837979	12.91%	4.892%
71	12.301	3406	3409	3411	rBV2	390	252	0.00%	0.001%
72	12.330	3411	3418	3429	rVB3	2375	3725	0.06%	0.022%
73	12.394	3431	3438	3440	rBV3	901	1013	0.02%	0.006%
74	12.523	3474	3478	3480	rBV2	543	403	0.01%	0.002%
75	12.674	3519	3525	3529	rBV4	473	556	0.01%	0.003%
76	12.832	3571	3574	3578	rBV	231	255	0.00%	0.001%

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 Title : VOC Analysis

77	12.902	3591	3596	3599	rVV2	280	263	0.00%	0.002%
78	13.137	3664	3669	3679	rBV5	649	1232	0.02%	0.007%
79	13.359	3732	3738	3742	rBV3	582	753	0.01%	0.004%
80	13.433	3754	3761	3769	rBV5	3056	4978	0.08%	0.029%
81	13.590	3801	3810	3820	rVV4	3532	5254	0.08%	0.031%
82	13.668	3831	3834	3836	rBV3	420	284	0.00%	0.002%
83	13.713	3844	3848	3853	rBV3	374	337	0.01%	0.002%
84	13.889	3900	3903	3905	rBV2	464	312	0.00%	0.002%
85	14.005	3929	3939	3949	rBV5	2292	3685	0.06%	0.022%
86	14.092	3962	3966	3973	rBV3	1923	2187	0.03%	0.013%
87	14.195	3988	3998	4013	rVB6	3546	6265	0.10%	0.037%
88	14.272	4020	4022	4027	rVB3	804	617	0.01%	0.004%
89	14.378	4049	4055	4058	rBV4	753	991	0.02%	0.006%
90	14.455	4070	4079	4085	rVB3	5135	6808	0.10%	0.040%
91	14.481	4085	4087	4091	rBV2	521	382	0.01%	0.002%
92	14.523	4097	4100	4105	rVB4	1164	851	0.01%	0.005%
93	14.574	4113	4116	4122	rVB5	2442	2368	0.04%	0.014%
94	14.645	4131	4138	4140	rBV4	1437	1464	0.02%	0.009%
95	14.925	4223	4225	4228	rBV3	506	247	0.00%	0.001%
96	14.947	4228	4232	4233	rBV	855	638	0.01%	0.004%
97	15.214	4309	4315	4327	rVB7	4344	7948	0.12%	0.046%
98	15.404	4368	4374	4383	rBV5	4517	6120	0.09%	0.036%
99	15.507	4401	4406	4408	rBV3	1333	1120	0.02%	0.007%
100	16.294	4645	4651	4660	rBV5	4282	5826	0.09%	0.034%

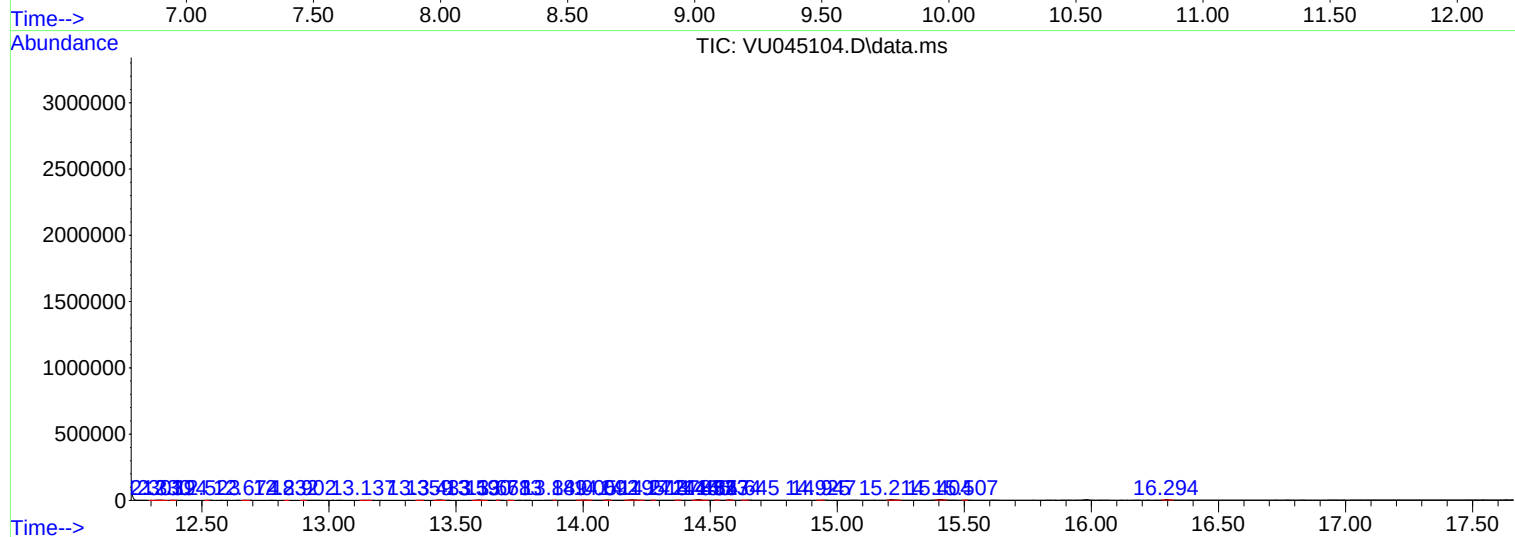
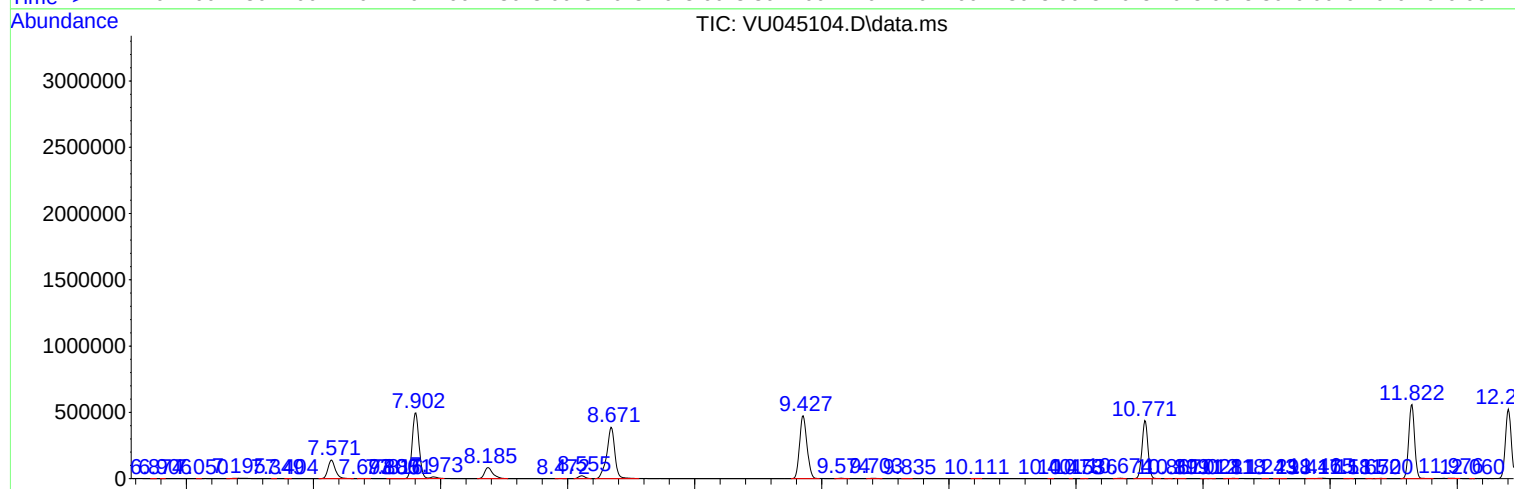
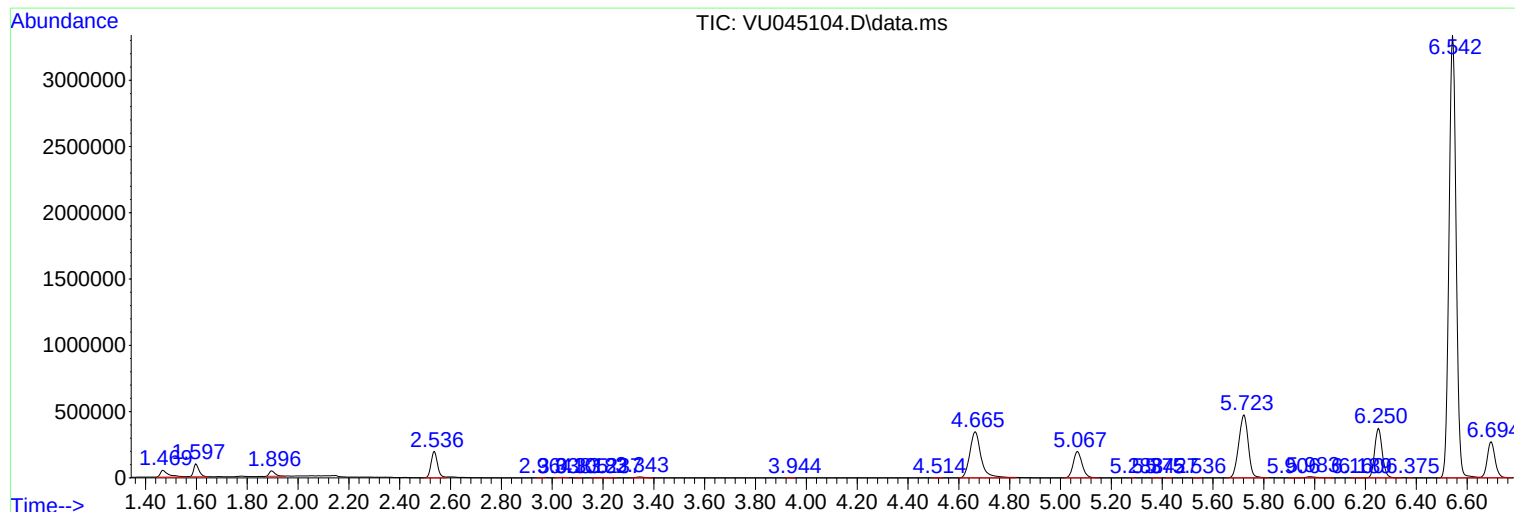
Sum of corrected areas: 17129523

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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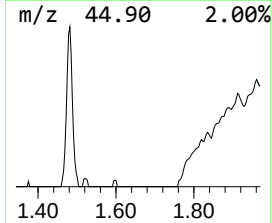
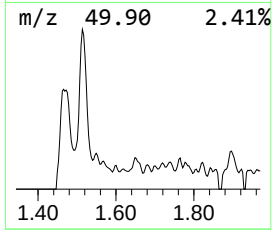
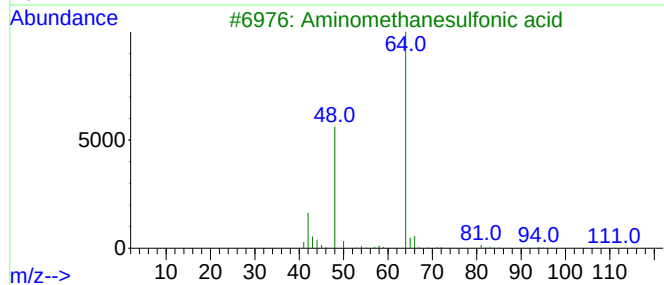
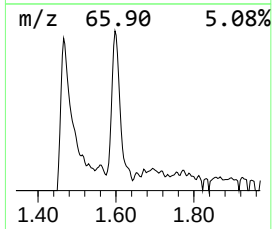
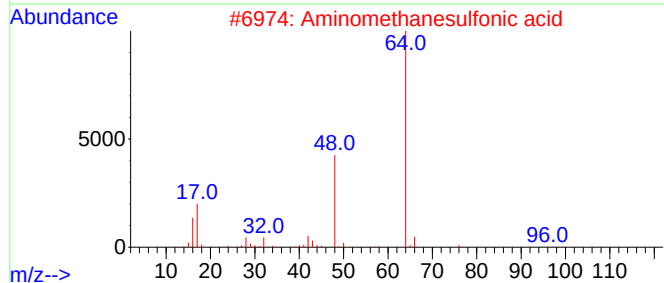
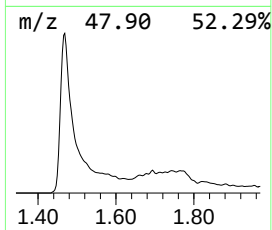
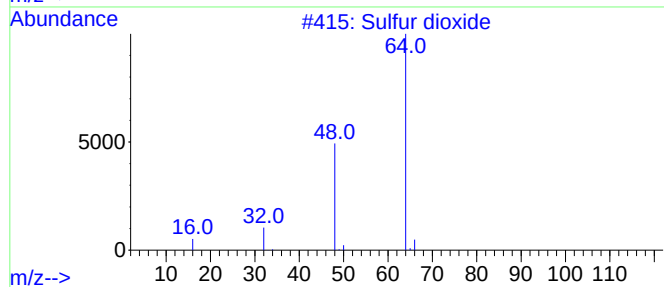
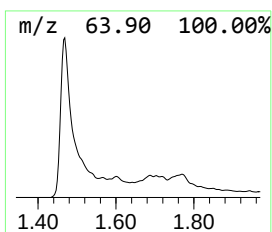
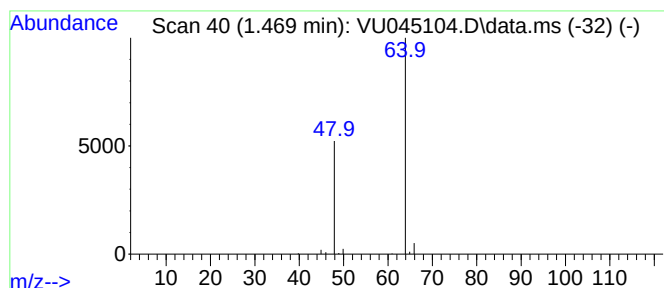
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	7.53 ug/L	116301	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	7.5	ug/L	116301	1	6.250	772461	50.0